

Species Tag:	51007	Species Name:	HCCNC-v5
Version:	1		Ethynyl-isocyanide,
Date:	Jan. 1995		ν_5 vibrational state
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	278	Q(300.0)=	3775.7021
Freq. (GHz) <	985.34	Q(225.0)=	2832.7507
Max. J:	99	Q(150.0)=	1888.7322
LOGSTR0=	-10.0	Q(75.00)=	944.7917
LOGSTR1=	-100.0	Q(37.50)=	472.8781
Isotope Corr.:	0.0	Q(18.75)=	236.9363
Egy. (cm ⁻¹) >	634.0	Q(9.375)=	118.9708
μ_a =	2.93	A=	
μ_b =		B=	4970.517
μ_c =		C=	

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. **156**, 39. The ν_5 vibration is the lowest excited bending state at 634 cm⁻¹. It should be noted that the ν_5 is an l doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. **30**, 1644.